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Title: MCNP6 Code Developments and CGMF/FREYA Integration and Validation

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MCNP6 Code Developments and CGMF/ FREYA Integration and Validation

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NA-22 Project Review

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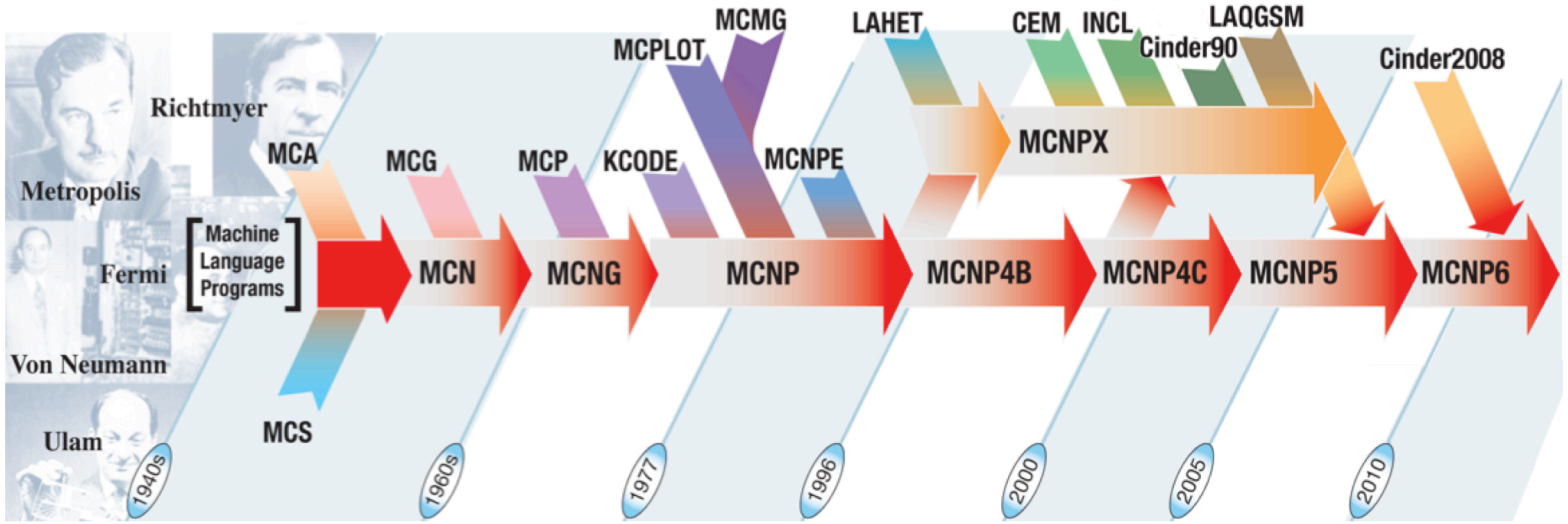
Outline

- **Background on MCNP6**
- **Release of MCNP6.2**
  - With CGMF & FREYA
  - With New Utilities
- **Ongoing Validation Efforts**
- **Code Modernization**
- **Conclusions & Upcoming Work**

Background of MCNP6

- **The history of MCNP can be traced back to the early days of LANL**



- **MCNP 6.1.0 released by RSICC in July 2013**

  MCNP6.1 + MCNP5-1.60 + MCNPX-2.70

  Nuclear Data Libraries + MCNP Reference Collection

- **MCNP 6.1.1 Update in July 2014**
- **MCNP 6.2.0 release to RSICC in April 2018**
- **MCNP5 & MCNPX are frozen – no future releases**

Release of MCNP6.2 (see mcnp.lanl.gov)

MCNP6.2 Release Notes and Manual

Release Information for MCNP6.2 Release

C.J. Werner, J.S. Bull, C.J. Solomon, et al.,,"MCNP6.2 Release Notes", LA-UR-18-20808 (2018).

C.J. Werner (editor), "MCNP Users Manual - Code Version 6.2", LA-UR-17-29981 (2017).

J.S. Bull, "How to Build MCNP6.2", LA-UR-17-30373 (2017).

MCNP Team,"MCNP6.2.0 Release Testing", LA-UR-17-29011 (2017).

F.B. Brown, M.E. Rising, J.A. Alwin, "Release of MCNP6.2 & Whisper-1.1 - Guidance for NCS Users", ANS 2017 Nuclear Criticality Safety Division Topical Meeting, Carlsbad, NM, LA-UR-17-24260 (2017)

F.B. Brown, M.E. Rising, J.L. Alwin, "What's New with MCNP6.2 & Whisper-1.1", LA-UR-17-27992(2017)

F.B. Brown, M.E. Rising, J.L. Alwin, "Verification of MCNP6.2 for Nuclear Criticality Safety Applications", ANS 2017 Winter meeting, Washington DC, Trans. ANS 117, LA-UR-17-24406 (2017).

F.B. Brown, M.E. Rising, J.L. Alwin, "Verification of MCNP6.2 for Nuclear Criticality Safety Applications", LA-UR-17-23822 (2017).

"Listing of Available ACE Data Tables", LA-UR-17-20709 (2017).

Data Changes for the MCNP6.2 Release, LA-UR-17-21486, LA-UR-17-20703

New Utilities

C.J. Solomon, C. Bates, J. Kulesza, "The MCNPTools Package: Installation and Use", LA-UR-17-21779 (2017).

C.J. Solomon "The Intrinsic Source Constructor Package: Installation and Use", LA-UR-17-22234 (2017).

C.J. Solomon "MCNP Intrinsic Source Constructor (MISC): A Users Guide", LA-UR-12-20252 (2012).

2017 NA-22 Collaboration Meeting

M.E. Rising, "MCNP6.2 Status & Developments: FY16 and early FY17", 2017 NA-22 Collaboration Meeting, Santa Fe, NM, LA-UR-17-21962 (2017)

Release of MCNP6.2

- **First item in the MCNP6.2 Release Notes, LA-UR-18-20808**

LA-UR-18-20808

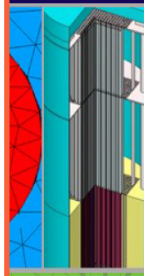
MCNP®

Release Notes

2.1 PHYSICS

2.1.1 Correlated prompt fission neutron and gamma-ray emission models (CGMF & FREYA):

Two new correlated fission event generators, CGMF and FREYA, have been integrated into the code to address needs within the nuclear nonproliferation and safeguards communities for high fidelity models of the neutron and gamma-ray emissions from both spontaneous and neutron-induced fission processes [2]. The ultimate use of these models, currently under active development at LANL and Lawrence Livermore National Lab/Lawrence Berkley National Lab, respectively, is to provide a predictive capability in simulating the unique signatures of special nuclear materials in situations where multiple detectors may be used in time-coincidence resulting in correlated counts from fission events. The new fission models can only be used for fixed-source calculations and are turned on with the FMULT card using the METHOD keyword.



Ongoing Validation Efforts (MCNP developer maintained, automated suites)

Verification Suites

- **REGRESSION**
  - Run by developers for QA checking
- **VERIFICATION_KEFF**
  - Analytic benchmarks, exact solutions for k_{eff}
  - Continuous-energy & multigroup
- **VERIFICATION_GENTIME**
  - 10 benchmarks for reactor kinetics parameters
- **KOBAYASHI**
  - 6 void & duct streaming problems, with point detectors, exact solutions
- **Ganapol Benchmarks**
  - Exact, semi-analytic benchmark problems
  - Fixed source, not criticality
- **Gonzales Benchmark**
  - Exact analytic benchmark with elastic scatter, including free-gas scatter

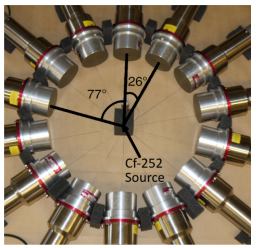
Validation Suites

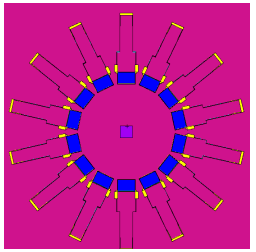
- **VALIDATION_CRITICALITY**
  - 31 ICSBEP Cases, too small for serious V&V
  - Today, used for
    - **Code-to-code verification, with real NCS problems & data**
    - **Compiler-to-compiler verification, with real NCS problems & data**
    - **Timing tests for optimizing MCNP coding & threading**
  - Run at least weekly, to check MCNP6 for NCS
- **VALIDATION_CRIT_EXPANDED**
  - 119 ICSBEP Cases
  - Broad-range validation, for developers
- **VALIDATION_CRIT_WHISPER**
  - 1101 ICSBEP Cases
  - Used with Whisper methodology for serious validation

Ongoing Validation Efforts

- **MCNP has historically had extensive verification and validation**
  - **Need to extend and leverage this work for correlated fission multiplicity applications**
- **Over the past 1-2 years, this important validation work for the correlated fission models has been getting started**
- **MCNP6.2 and MCNPX/PoliMi code-to-code comparison**
  - Not really verification or validation
  - Help in understanding differences in codes
- **Creating an automated subcritical benchmark test suite**
  - Validation with evaluated benchmark quantities
- **Using the criticality benchmark test suites**

Ongoing Validation Efforts
MCNP6.2 – MCNPX/PoliMi Comparisons

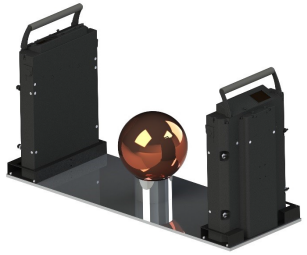




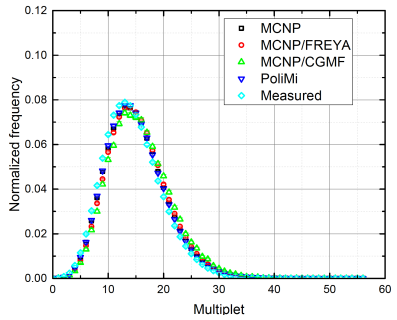
- **Follow-up of 2014 NSE paper by S.A. Pozzi *et al*.**
- **Presented at 2017 IRRMA X (LANL-UM collaboration)**
  - "Correlated Fission Simulations with MCNP6.2 and MCNPX-PoliMi", M.E. Rising, M.T. Andrews, M.J. Marcath, A. Sood, S.D. Clarke and S.A. Pozzi
- **MCNP6.2 Simulations**
  - Binary PTRAC file written and processed by DRiFT using MCNPtools
  - Convert PTRAC using MCNPtools for MPPost code detector response
- **MCNPX-PoliMi Simulations**
  - Collision file used for MPPost code detector response processing
  - ASCII PTRAC file written and processed by DRiFT using MCNPtools
- **Count rates/pulse height spectra between transport codes and multiplicity models are consistent**

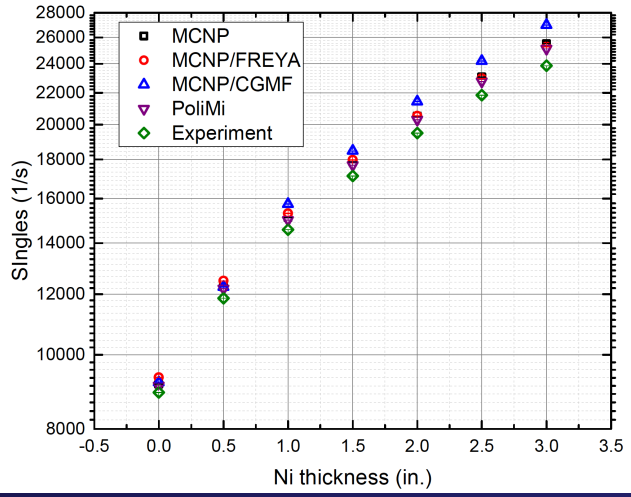
	Total Counts (#/fission)	Correlated Counts (#/fission)
Experimental rate	0.142	0.00439
Exp. light output threshold	64 keVee	100 keVee
DRiFT rates		
MCNP6.2, FMULT	0.211	0.0116
PoliMi, FMULT	0.212	0.0116
MCNP6.2, FREYA	0.209	0.0119
MCNP6.2, CGMF	0.212	0.0122
PoliMi, IPOL(1)=1	0.211	0.0121
PoliMi, IPOL(1)=10	0.211	0.0119
MPPost rates		
MCNP6.2, FMULT	0.138	0.00398
PoliMi, FMULT	0.138	0.00398
MCNP6.2, FREYA	0.141	0.00468
MCNP6.2, CGMF	0.143	0.00490
PoliMi, IPOL(1)=1	0.143	0.00461
PoliMi, IPOL(1)=10	0.141	0.00452
Sim. light output threshold	53 keVee	100 keVee

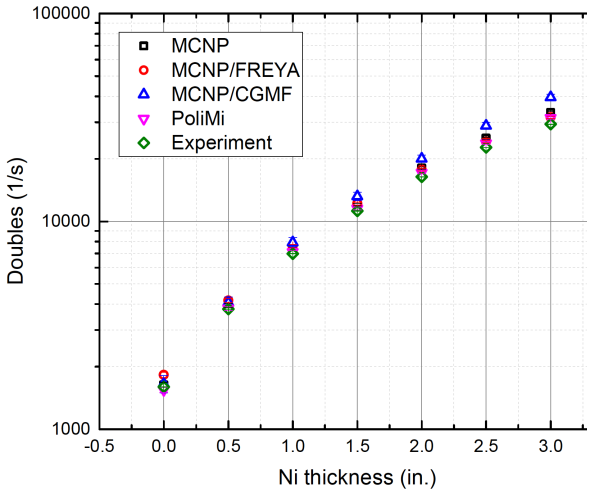
Ongoing Validation Efforts
Subcritical Benchmark Validation

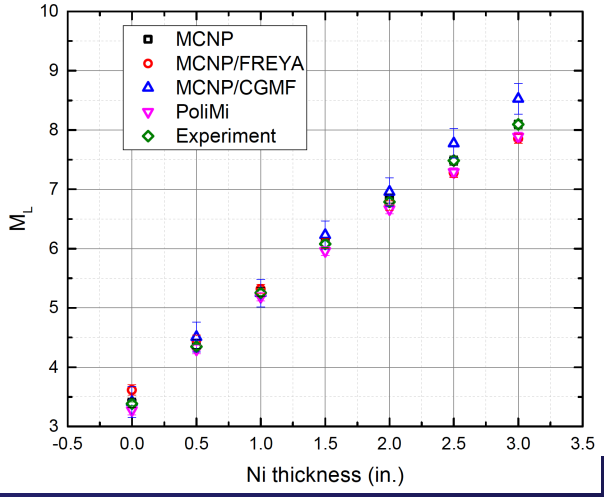


- **Leveraging benchmark quality subcritical experiments**
- **Two papers with lead author J.A. Arthur (CNEC Student)**
  - "Validating the performance of correlated fission multiplicity implementation in radiation transport codes with subcritical neutron multiplication benchmark experiments", Annals of Nuclear Energy
  - "Validation of MCNP6 Using Subcritical Benchmark Experiments", submitted to 2018 ANS ANTPC
- **These applications represent "integral" quantities that can be sensitive to the correlated multiplicity models**



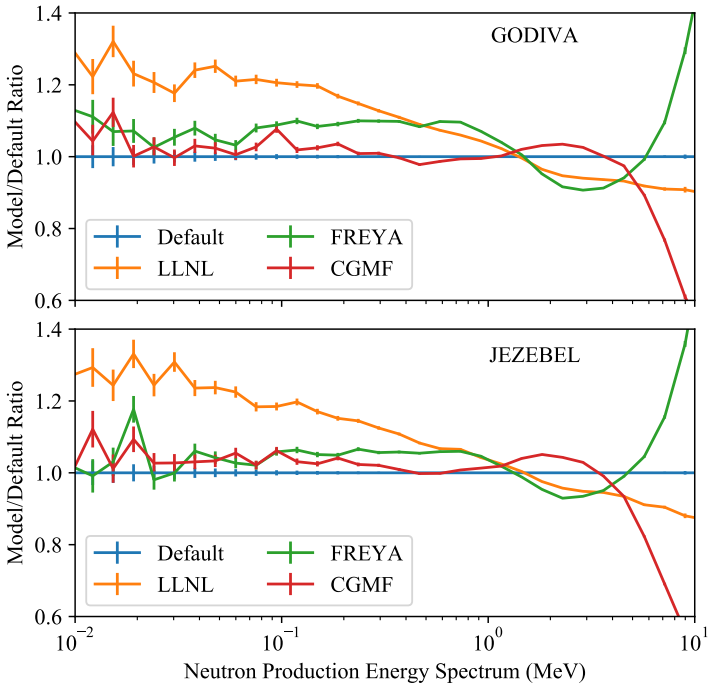






Ongoing Validation Efforts
Criticality Benchmark Validation

- **Leveraging benchmark quality criticality experiments**
- **One paper with lead author D. Timmons (UNM Student)**
  - "Evaluating the MCNP6.2 Correlated Fission Multiplicity Models for Criticality Calculations", submitted to 2018 ANS Winter Meeting
- **The default MCNP5/6 have been extensively validated for criticality safety applications**
- **MCNP6.2 disallows the use of the correlated fission multiplicity models in criticality safety because a serious lack of validation**
- **Using these models in criticality calculations is currently being investigated**



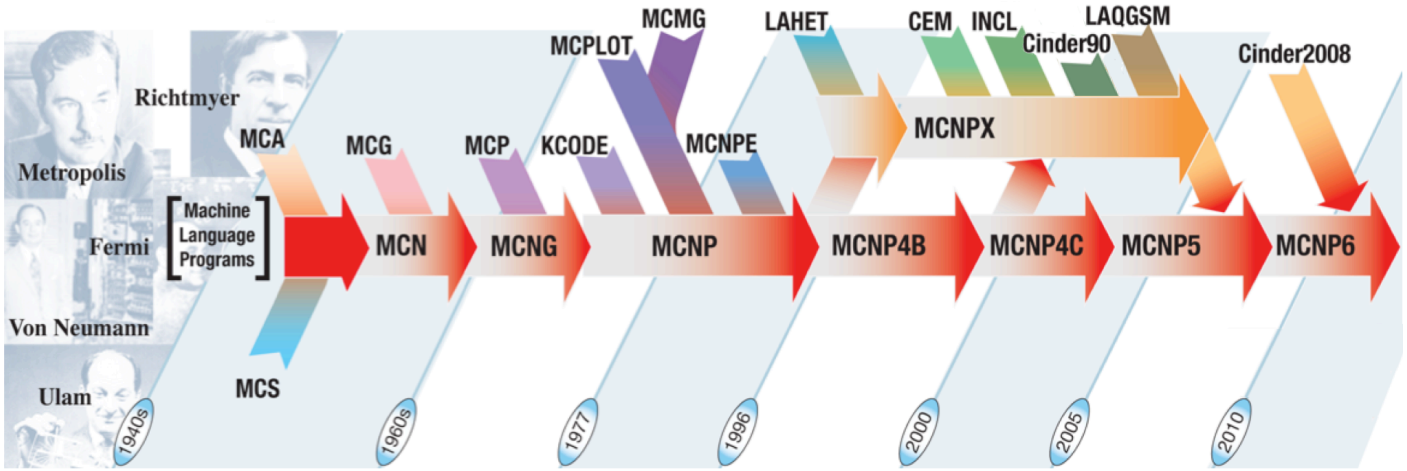
Model	GODIVA k_{eff}	JEZEBEL k_{eff}	FLAT23 k_{eff}	FLAT25 k_{eff}
Default	0.99987(19)	0.99987(19)	0.99915(30)	1.00331(30)
LLNL	0.99897(34)	0.99515(31)	0.99673(37)	1.00005(37)
FREYA	1.00053(34)	1.00097(31)	1.00121(39)	1.00568(37)
CGMF	0.99589(32)	0.99500(30)	0.99730(55)	0.99928(55)

Ongoing Validation Efforts

- **Part of the reason that MCNP has a reputation as the "gold standard" for many applications is because of the validation testing**
  - Constant and automated testing done by code developers
  - Regular reports issued on the validation test suite results
  - Changes to the code and nuclear data can be immediately tested
- **Critical and subcritical benchmark applications are being leveraged to test the correlated fission models**
  - These applications are relevant to the models
  - However, they are not highly sensitive to CGMF/FREYA
- **A new test suite dedicated to correlated fission model experiments would be a great addition to the MCNP testing repertoire**
  - Immediate feedback to the user community on application validity
  - Immediate feedback to the CGMF/FREYA developers on model improvements

Code Modernization

- **The state of MCNP6.2**
  - **The long (and occasionally windy) road to today**



- **Currently, the code base includes:**
  - 431K lines of code + 88K lines of comments ~ 500K total
  - ~ 9-10 FTE total primarily funded through ASC / NCSP / SC / Institutional

- **This is a big job for all of us**
  - Seeking the best and brightest new staff members, of course
  - Young staff are used to and expect more modern code practices!

Code Modernization

- **At LANL, there exists a strong will to see MCNP succeed**
- **How do we (curators of the code) setup for long term success?**
  - Create a code modernization plan (under development)
  - Improve code development practices as a team
    - Code design documentation and prototyping practices
    - Peer-review and testing of all integrated code
    - Complete documentation of all code work
    - With all of these improved team processes documented and in place leads to improved SQA
  - Adopt modern software development tools
    - ✓ Version control system – CVS ➔ git 
    - ✓ Build, test and package software – GNU Make ➔ CMake 
    - ✓ Repository management / code reviews – TeamForge / Gerrit ➔ Bitbucket 
    - ✓ Artifact / issue tracking – TeamForge ➔ Jira 
    - ✓ Team communication / wiki – TeamForge ➔ Confluence 
    - Continuous build and testing system – CBTS ➔ ???

ATLASSIAN

Code Modernization

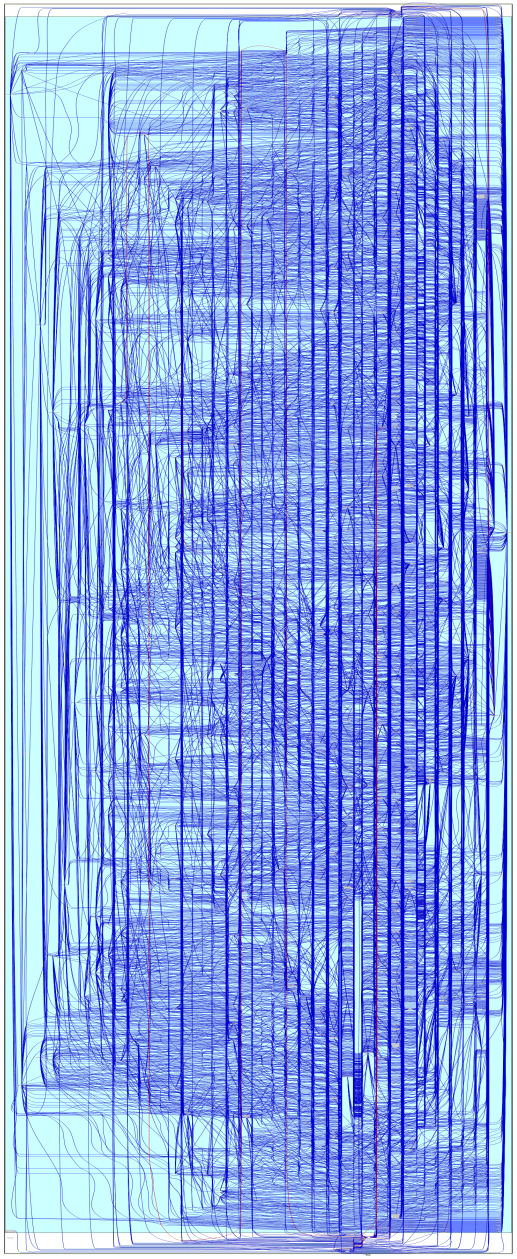
- **With all of the history of MCNP comes…**

… many benefits

- Very feature-rich, many applications possible
- Extensive testing (90% coverage of code)
- Validation for important applications (i.e. NCS)
- Expert experience and guidance available

… many challenges

- A tangled mess of source code, dependencies, etc. (see dependency graph ➔)
  - No modularity – need to break dependencies
  - Unintended side-effects when calling a function
- Diminished knowledge of some features
- Structural upgrades sorely needed
  - Remove cryptic variable naming (2-3 letter variables)
  - Organize data structures in a logical way



Code Modernization

- **How does the MCNP code modernization efforts impact this project?**
- **Examples from previous venture integration efforts**
  - CGMF now contains API to interact with MCNP
  - FREYA is now Fortran 2003 compliant
- **During current project (CGMF-specific)**
  - Using newer tools (git, Bitbucket, etc.)
  - Currently implementing CMake to replace build system
  - Will address automated testing soon
  - Include C/Fortran/Python interface
- **With these kinds of changes, the burden on MCNP developers to maintain external dependencies is reduced**

Conclusions & Upcoming Work

- **MCNP6.2 includes CGMF & FREYA!**
  - Documented in many places, with many links on website
  - Release notes and manual updated with correlated model info
  - New tools available to support users
- **Validation is essential**
  - Historically, MCNP focus on criticality and shielding applications
  - Need to expand validation suites to correlated fission multiplicity applications – ongoing & future work
- **MCNP6 is undergoing serious code modernization**
  - Maintain performance and validation
  - Need modern code for long-term sustainability
- **Need to improve parallelism and performance**

Questions?